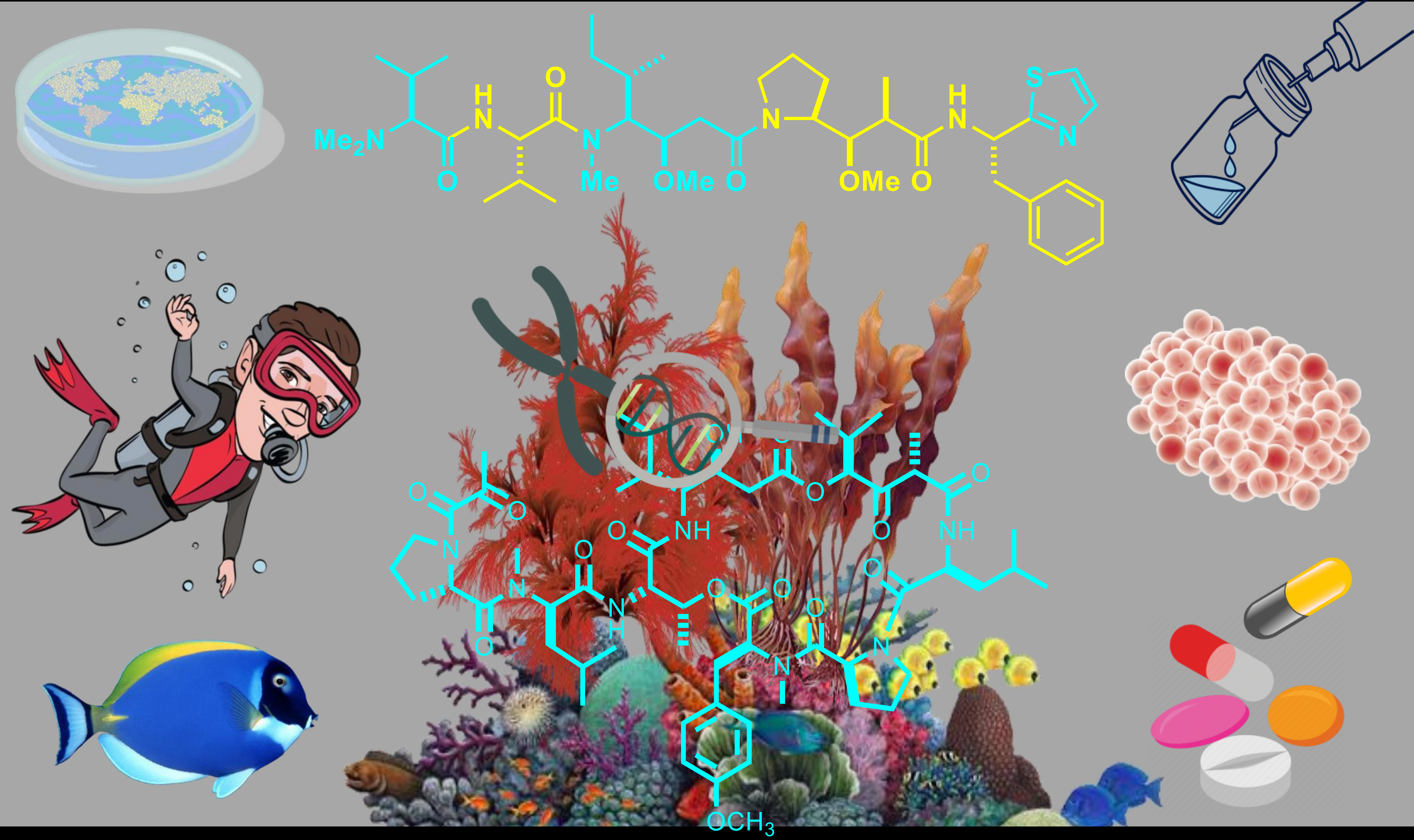
Marine Drugs



Dr. Omar M. Sabry

Marine Sample Collection

Marine Sample Collection

Shallow

Near Shores

More than 100 Feet

{Submarines}

Not more than

100 Feet {SCUBA}

Hand Snorkeling

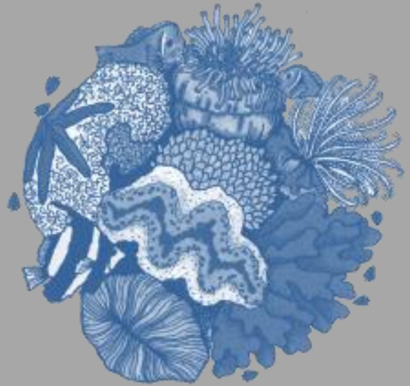
SCUBA

Marine Sample Collection

15 – 100 feet Depth

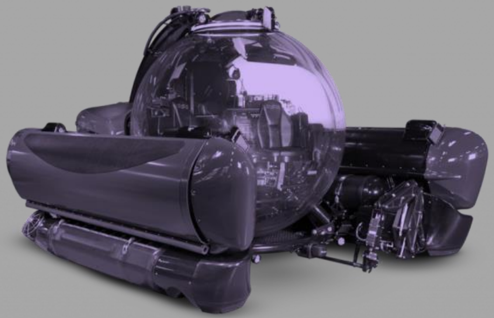
SCUBA

Marine Sample Collection



Shallow {5 – 15 feet}

Snorkeling



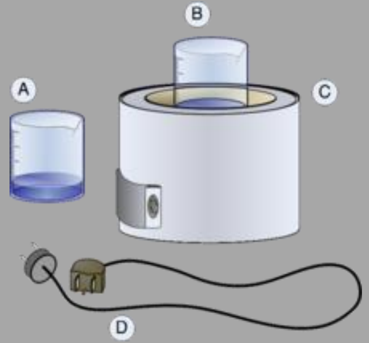
More than

100 feet Depth

Submarine

Why Extraction with Organic Solvents?

Size Reduction and Extraction



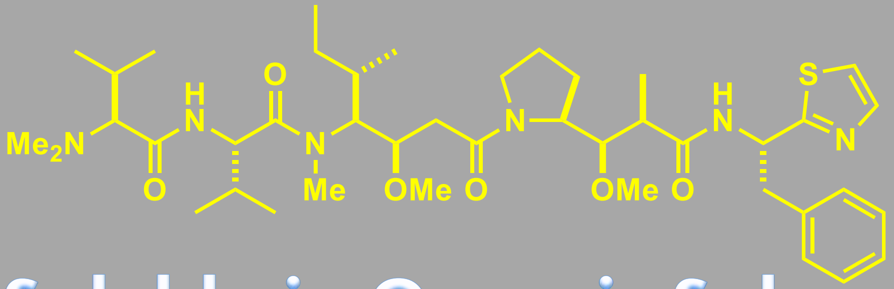
Not more than 30 0C

Organic Solvent

CH_3OH/CH_2Cl_2

Water

Bioactive Constituents



Soluble in Organic Solvents

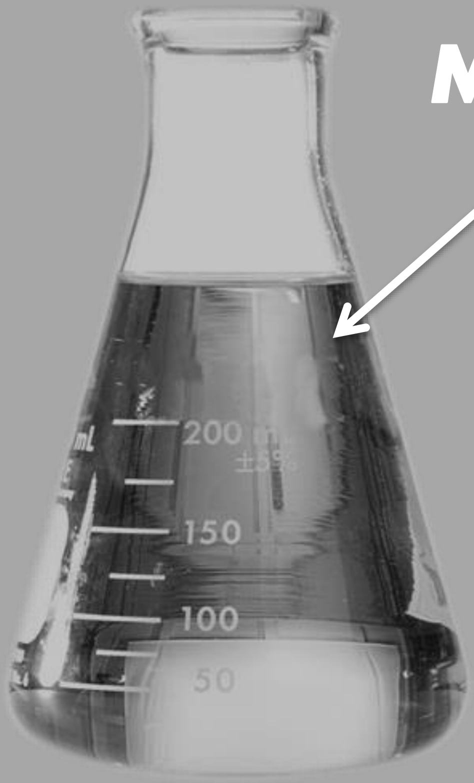
Bioactive Constituents Not Extracted

Extraction with Organic Solvents

Extraction with Organic Solvents

Sample

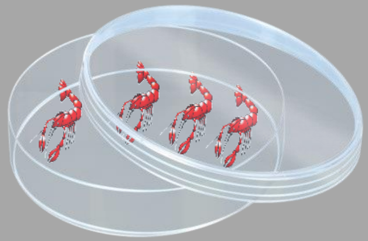
Size Reduction Extraction



Methanol, CH_2Cl_2 Solvent

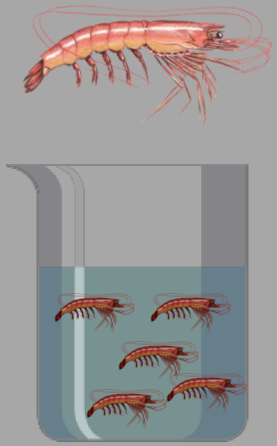
Extract

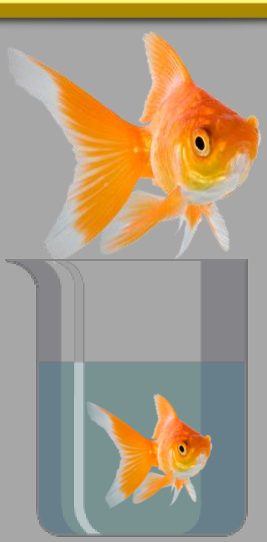
Preliminary Biological Screening



Preliminary Biological Screening

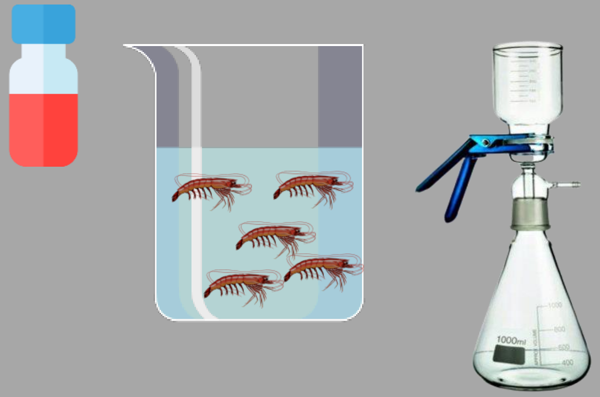
- **Brine Shrimp Toxicity**
- **Ichtyotoxicity Snail Killing**
- **GoldFish Toxicity**





Toxic Extract = Bioactive compound{s}

Bioassay-guided fractionation



Crude Extract
CH_3OH/CH_2Cl_2

Active

COX-II

Pseudopterogorgia elisabethae extract

Vacuum Liquid Chromatography

Pet. Ether

Pet. Ether/ Ethyl Acetate

Ethyl Acetate

Methanol

HPLC

Active

Compound 1

Compound 2

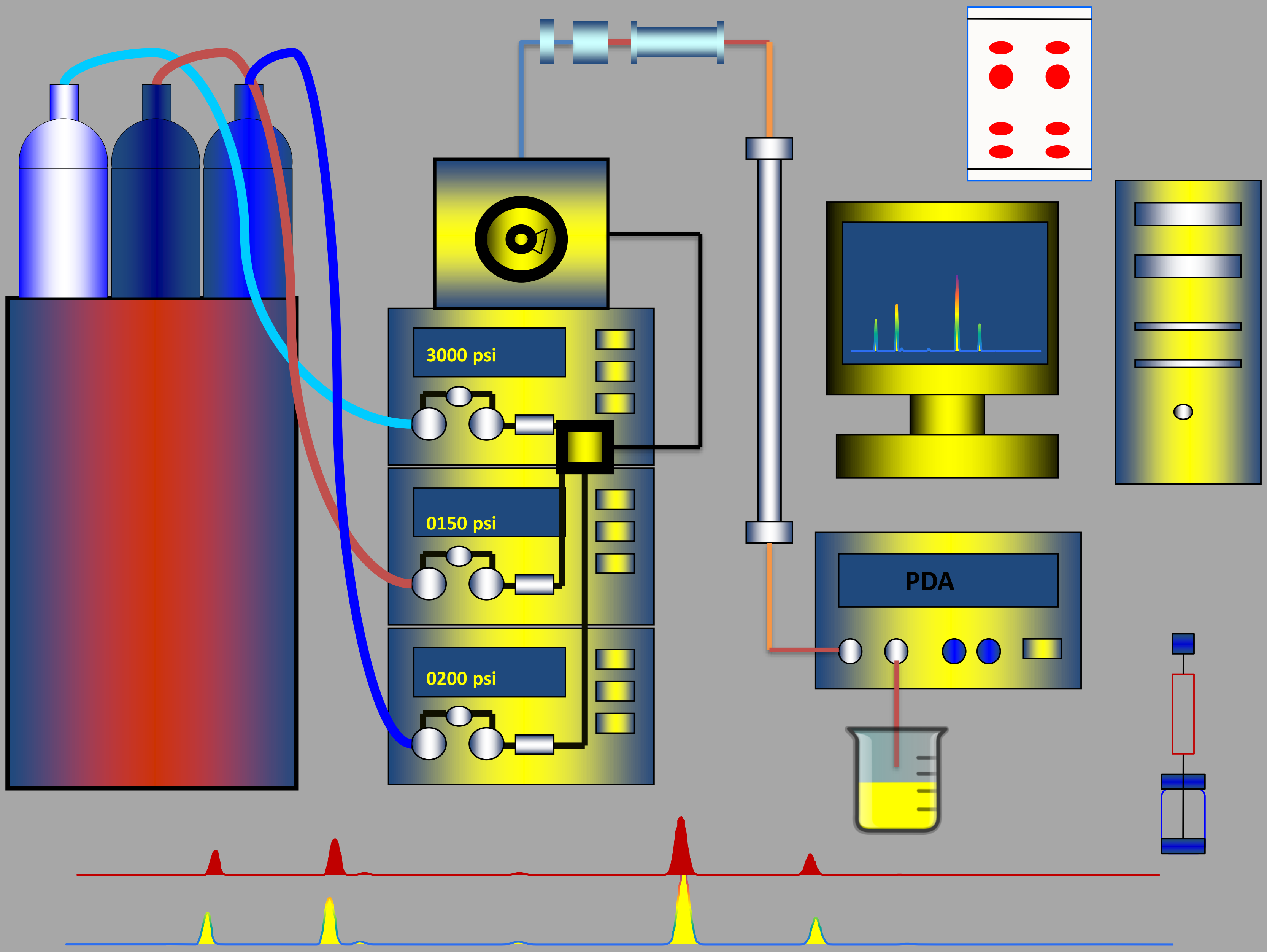
Compound 3

Compound 4

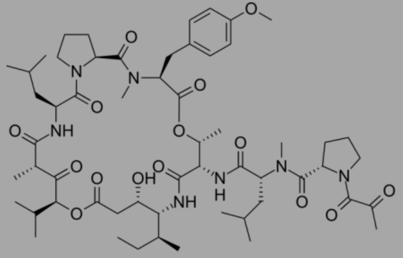
Active

Pseudopterosine A

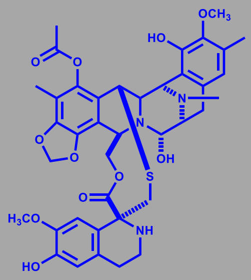
HPLC



Structural Elucidation of Bioactive Compounds



Compound



Elemental Analysis

UV UltraViolet

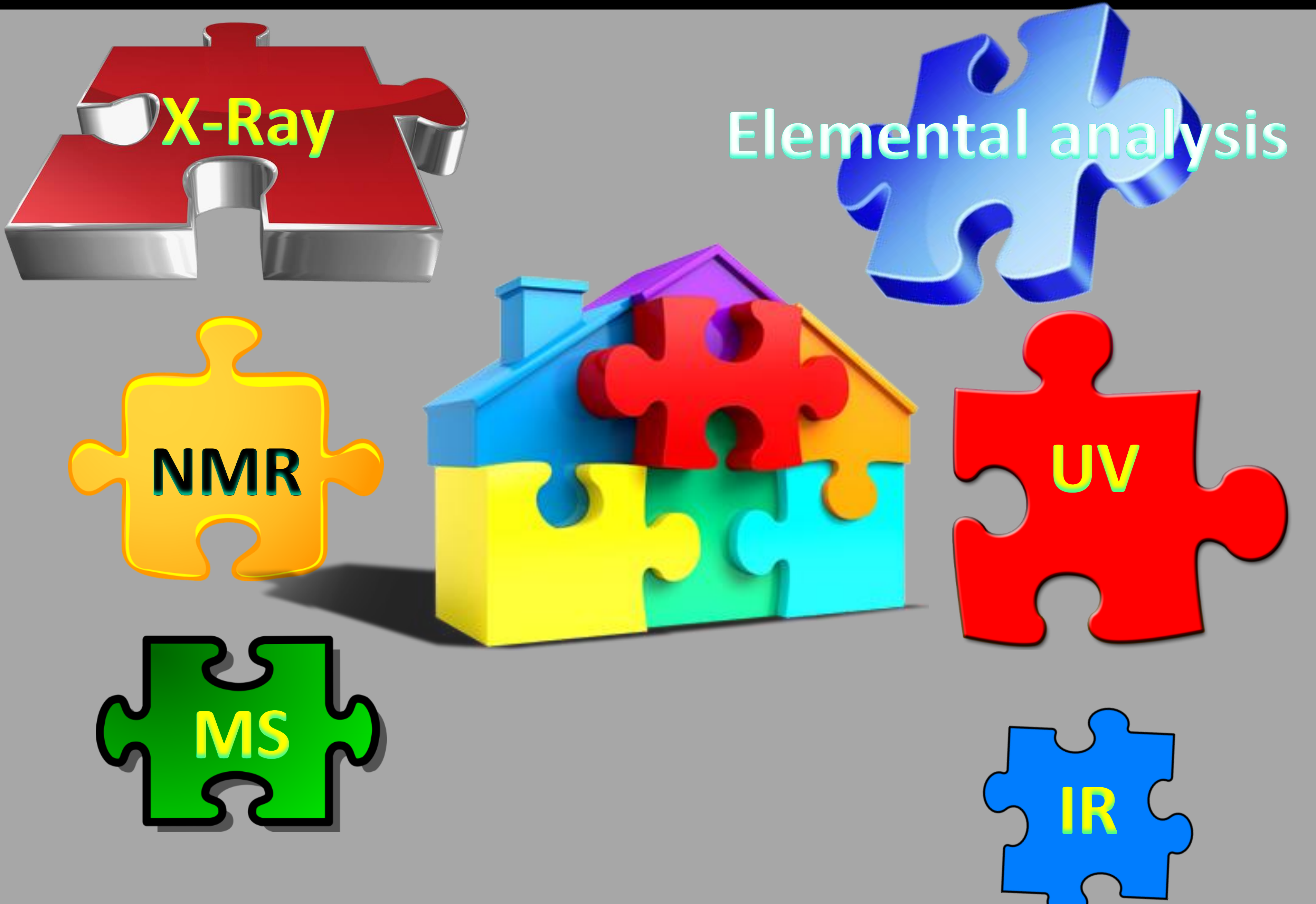
IR InfraRed

MS

NMR

X-Ray

Structural Elucidation



X-Ray

Elemental analysis

NMR

UV

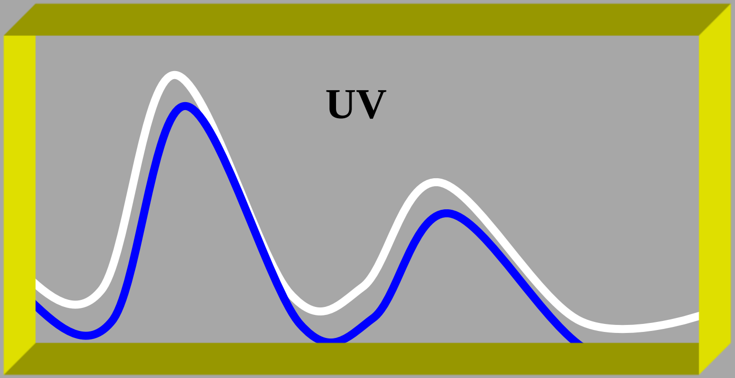
MS

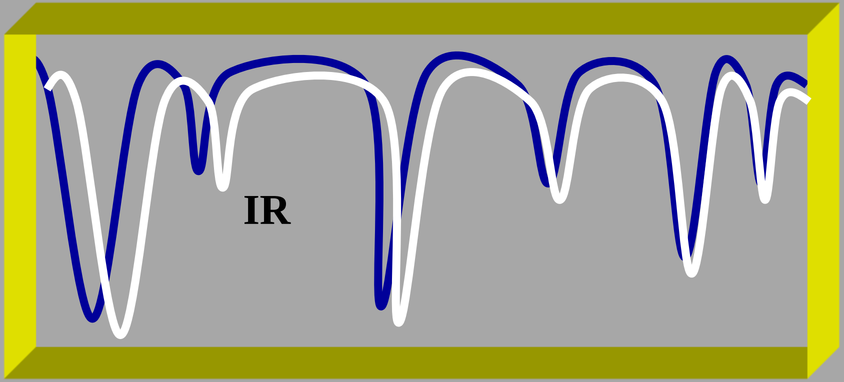
IR

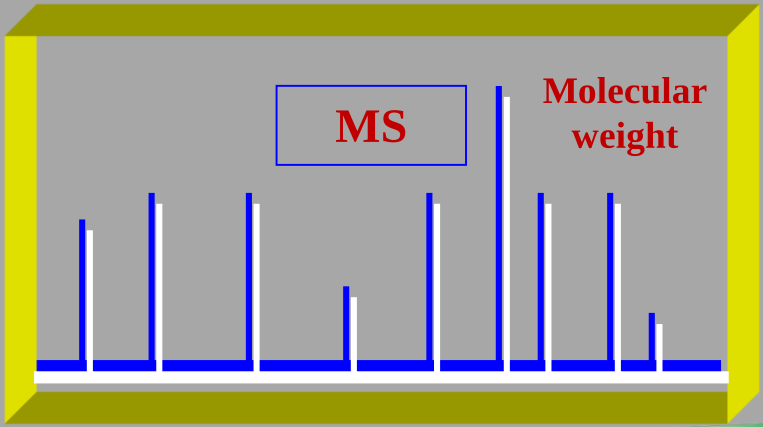
Structural Elucidation

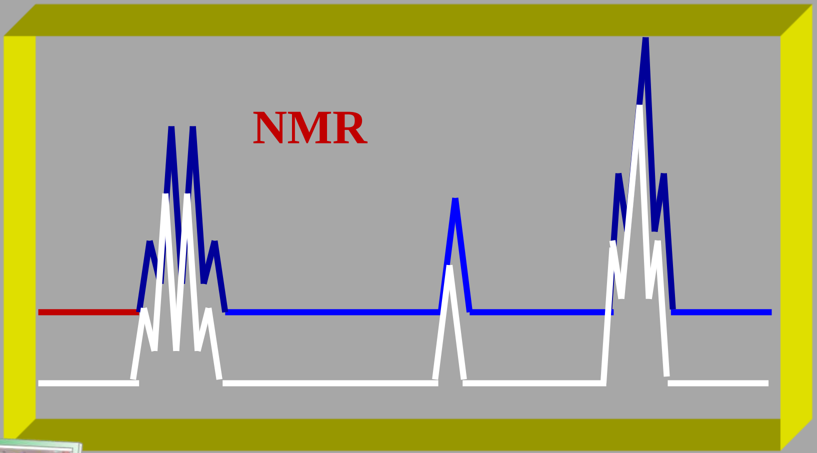
Elemental Analysis: C = 66.11; H = 6.02; N = 1.64; O = 26.23

Formula: $C_{47}H_{51}NO_{14}$ Mass: 853

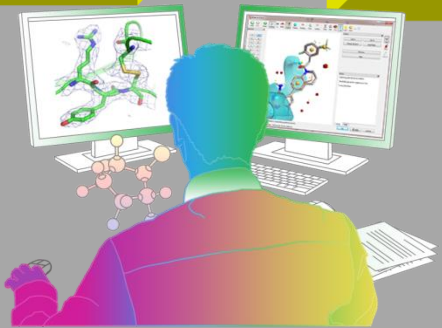


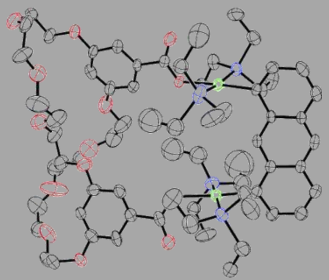




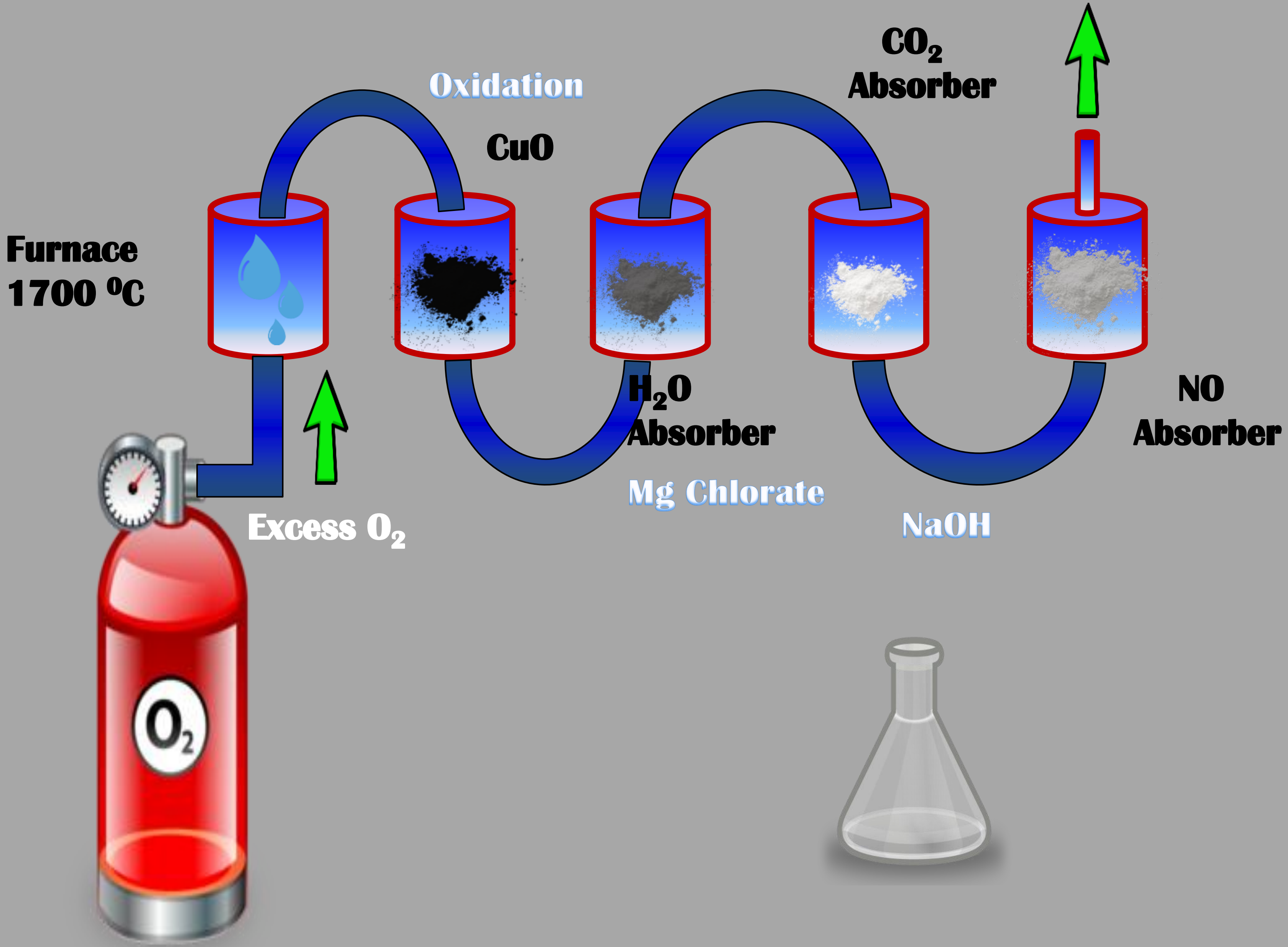


X-Ray





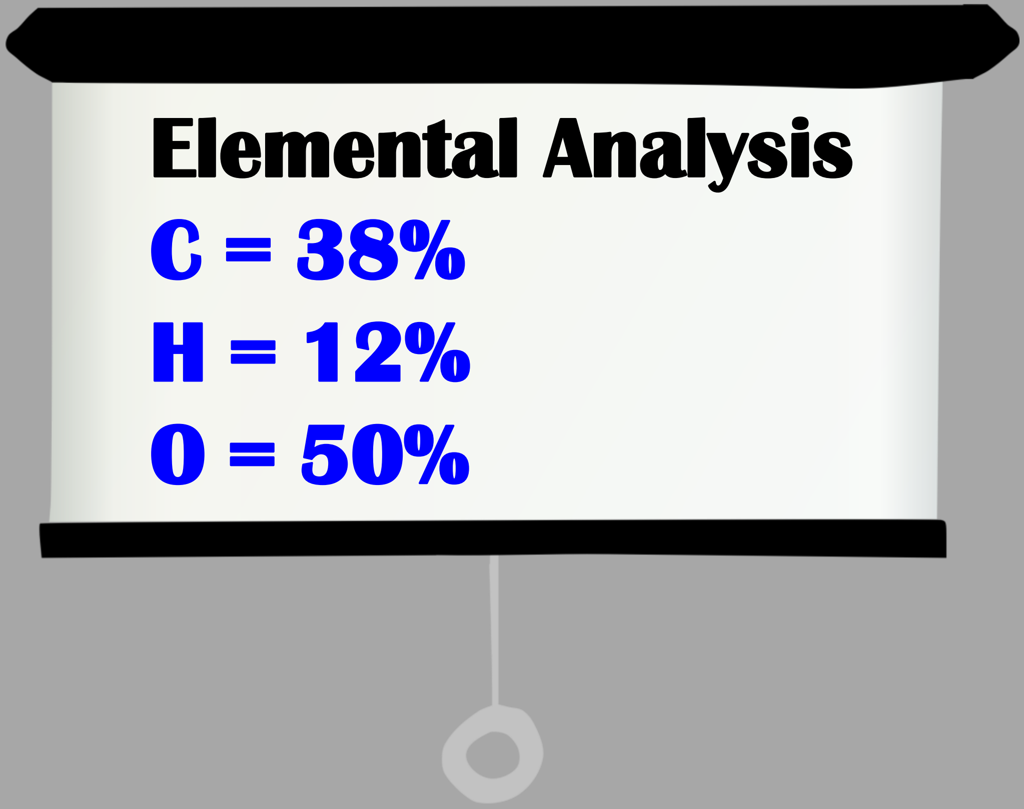
Elemental Analyzer



Elemental Analyzer

Determination of % C ,% O, % N and % H

Determine the Emperical formula $CH4O$



Elemental Analysis

C = 38%

H = 12%

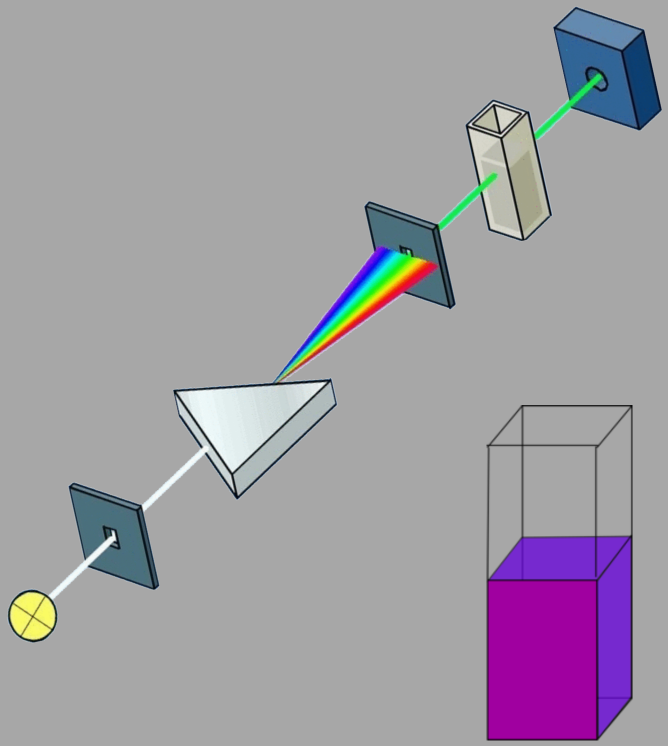
O = 50%

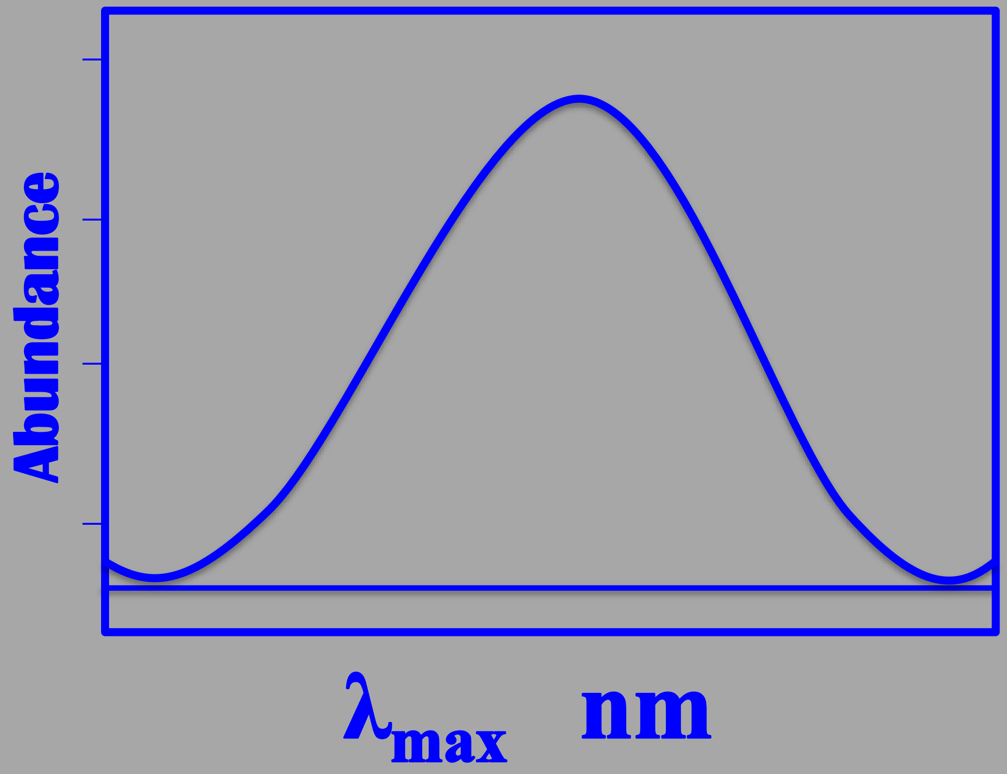
UV Spectroscopy

Electromagnetic waves

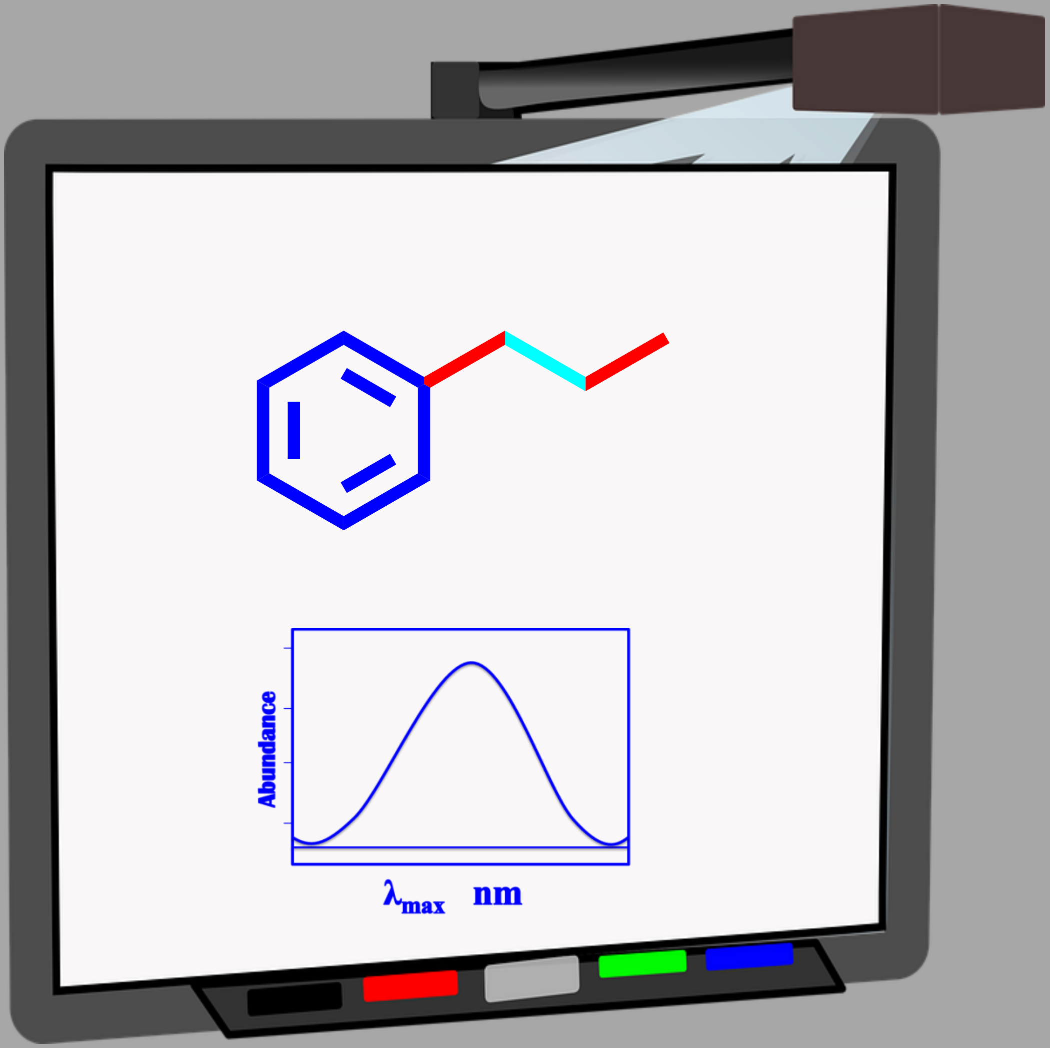
Range of wave length 200 - 400 nm.

Gives an idea about chromophores (conjugated double bonds, present or absent)



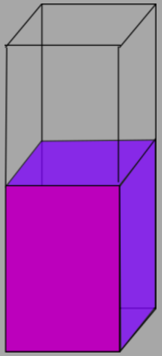


UV Spectroscopy



λ_{max}

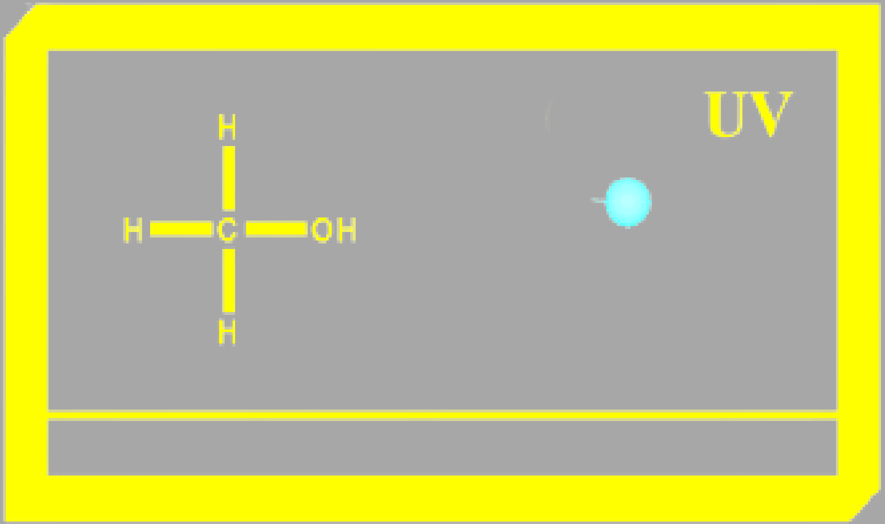
266 nm

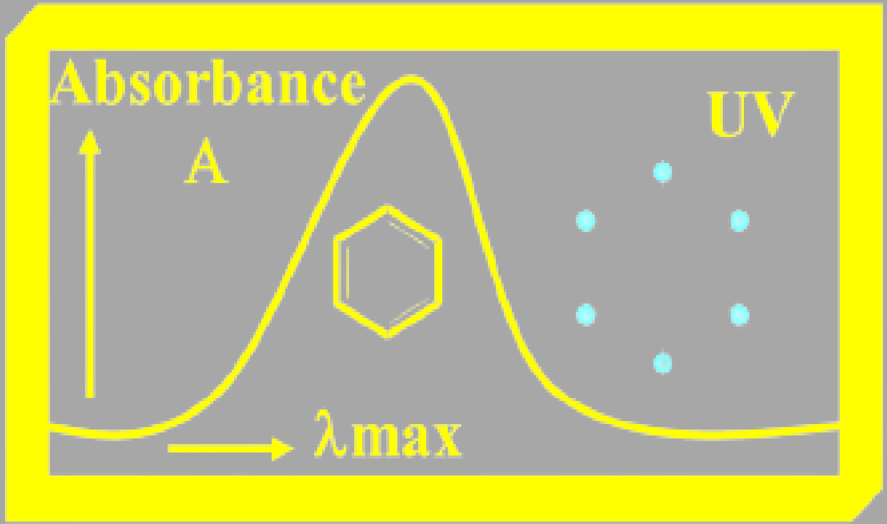


UV Spectroscopy

Compounds absorb at UV range

{Conjugated systems = Chromophores}



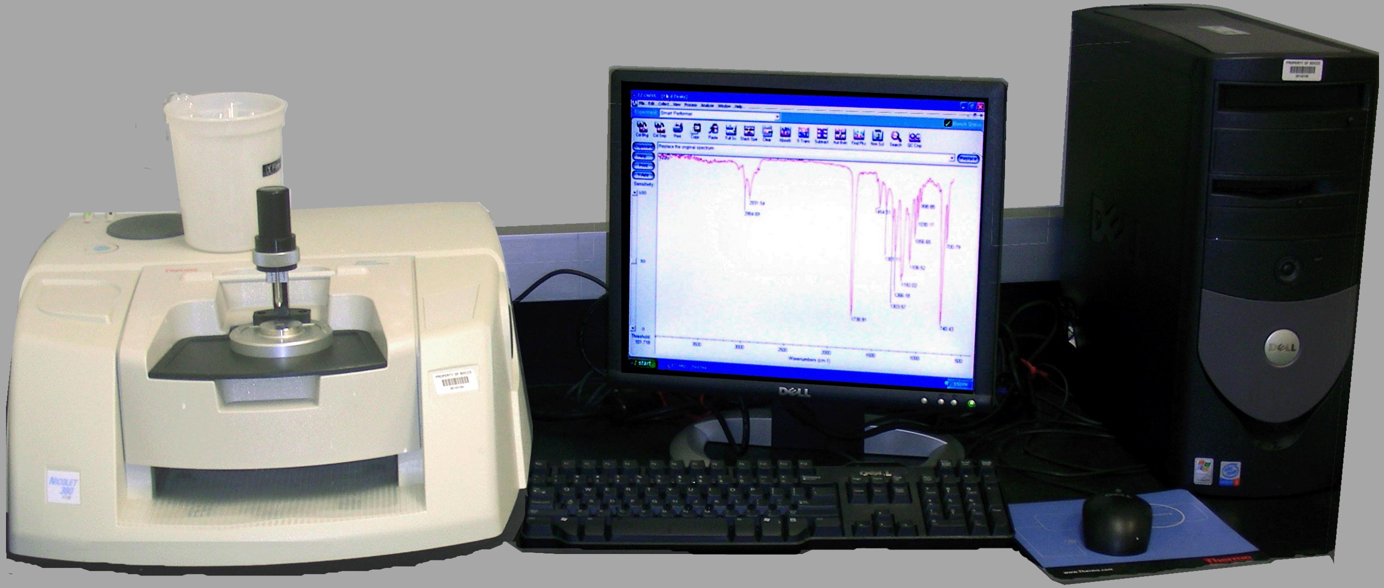


IR Spectroscopy

Gives an idea about:

Functional groups = Functional group region

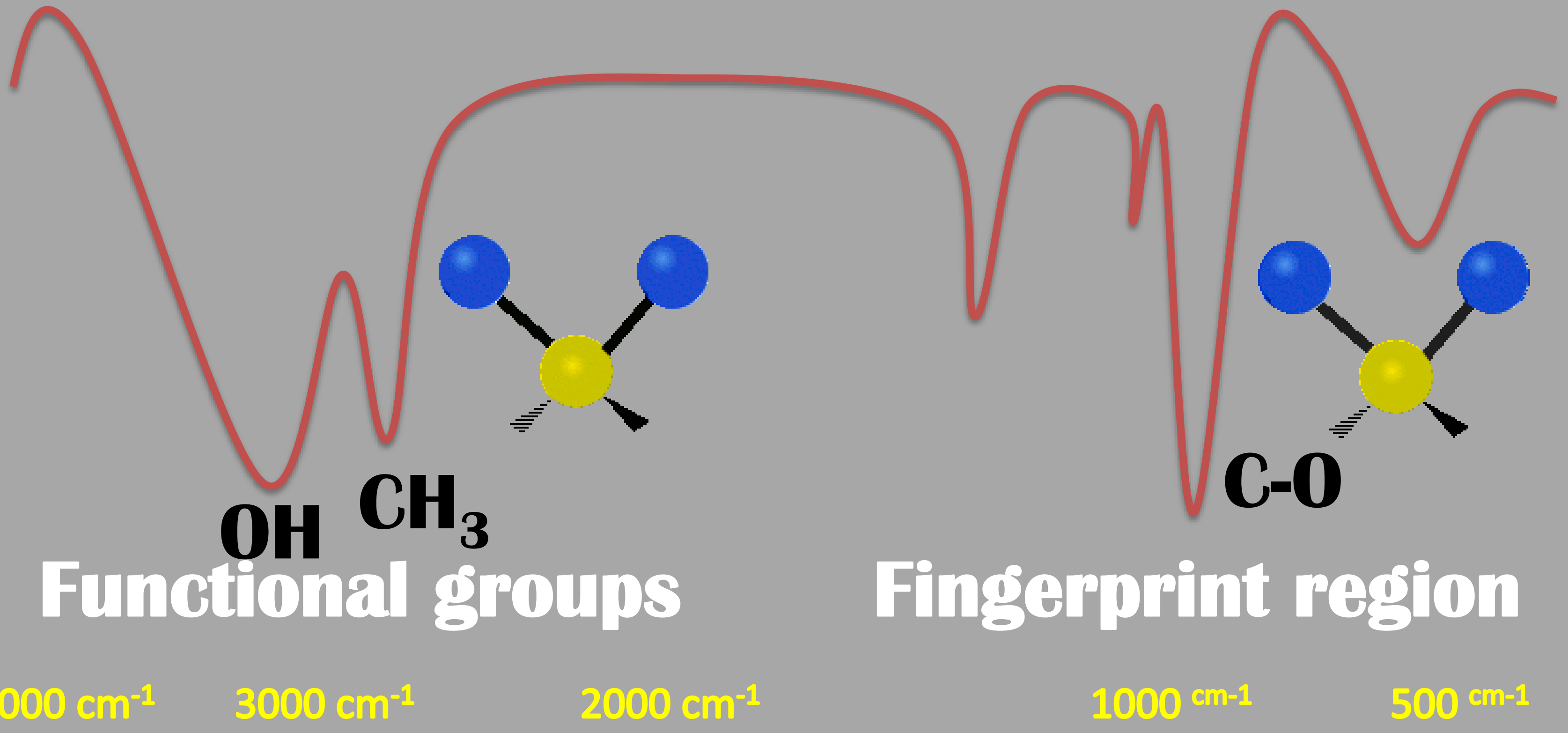
Nucleous = Fingerprint region



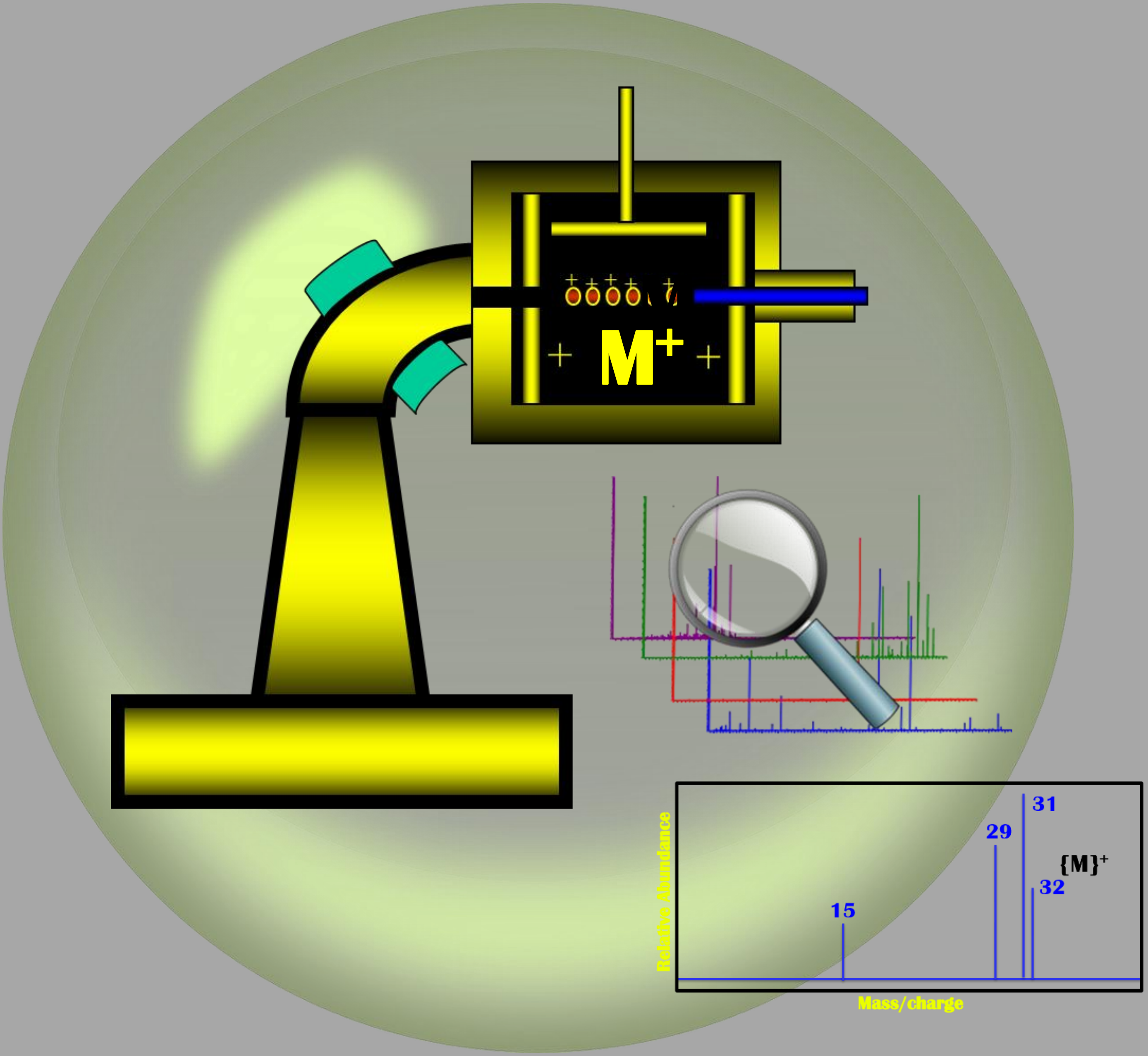
IR Spectroscopy

Functional groups = Functional group region

Nucleous = Fingerprint region



Mass Spectroscopy

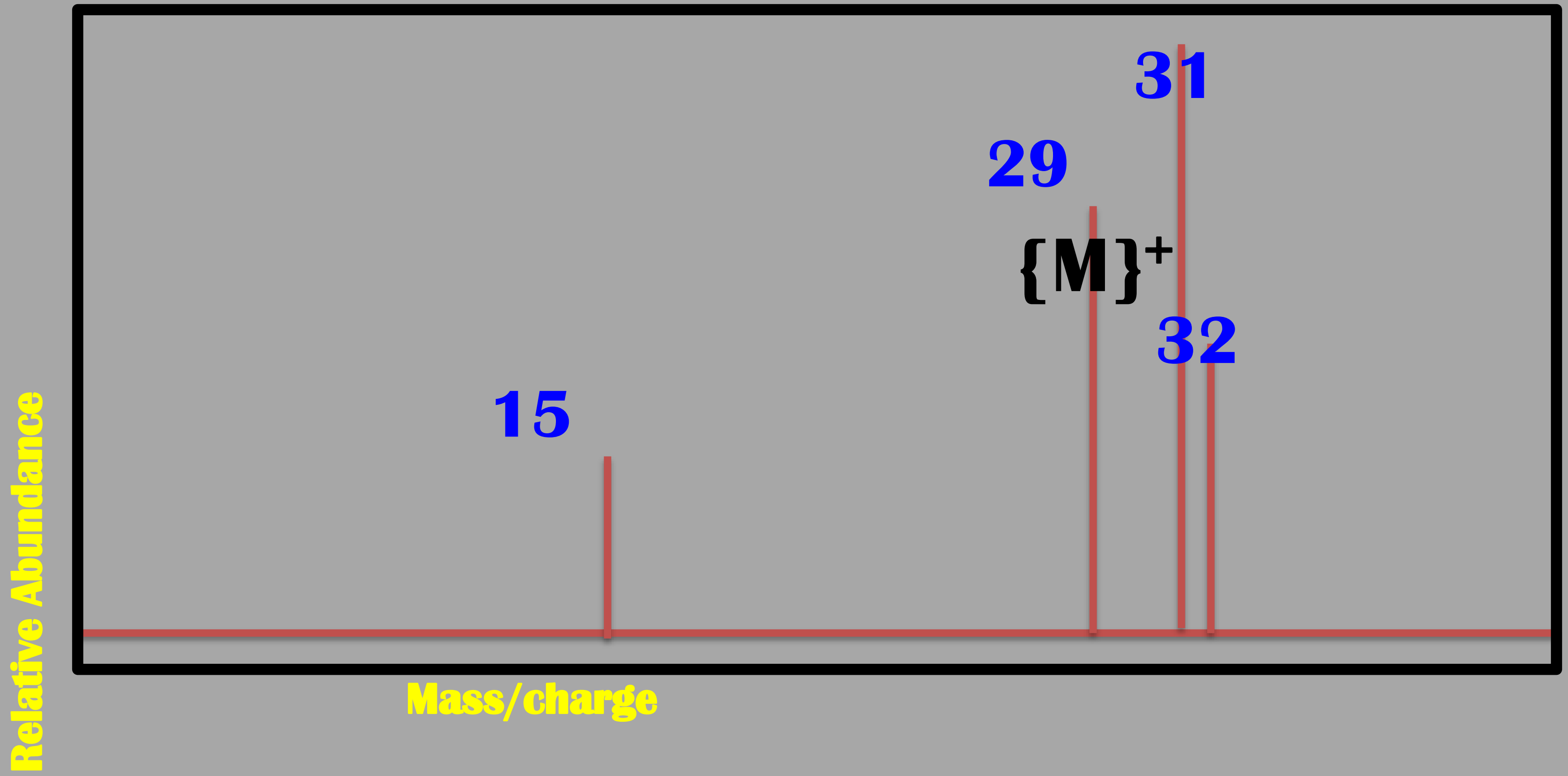


Mass Spectroscopy

Determines Molecular Weight Compound {M$^+$}

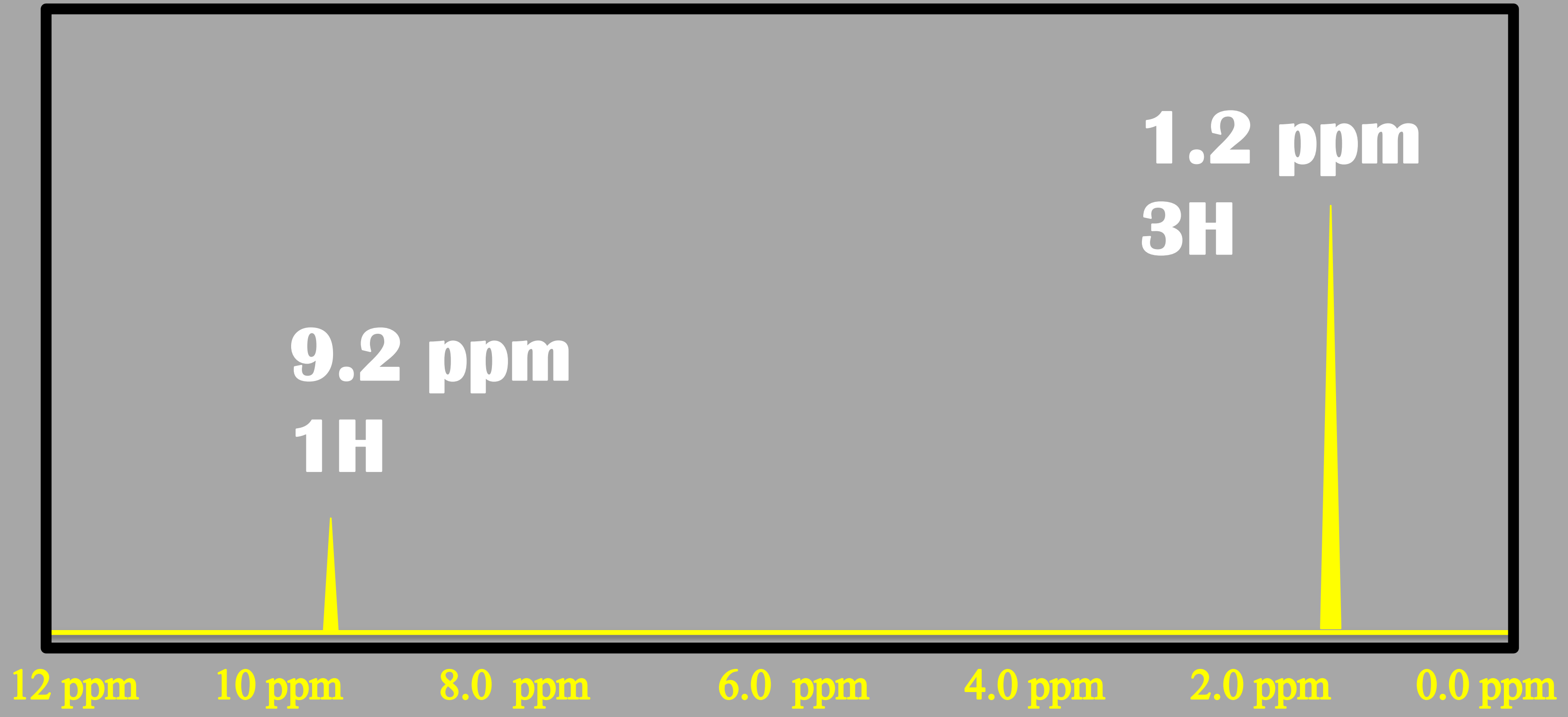
{High Resolution Mass Spectroscopy HRMS}

Molecular Formula



^{1}H-NMR

How many types of hydrogen are present?,
How many H of each type are there?

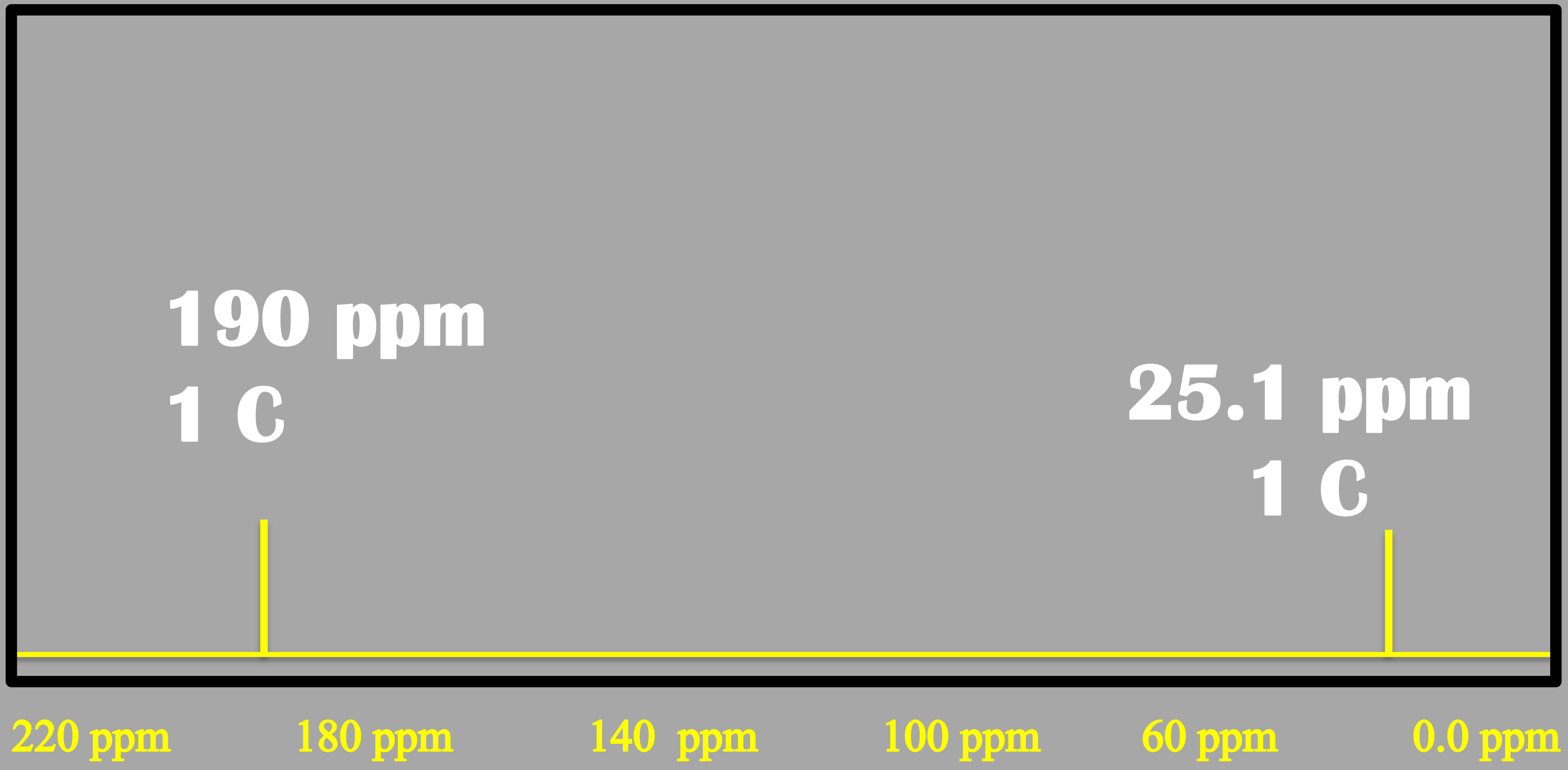


^{13}C-NMR

How many carbon are present in the molecule

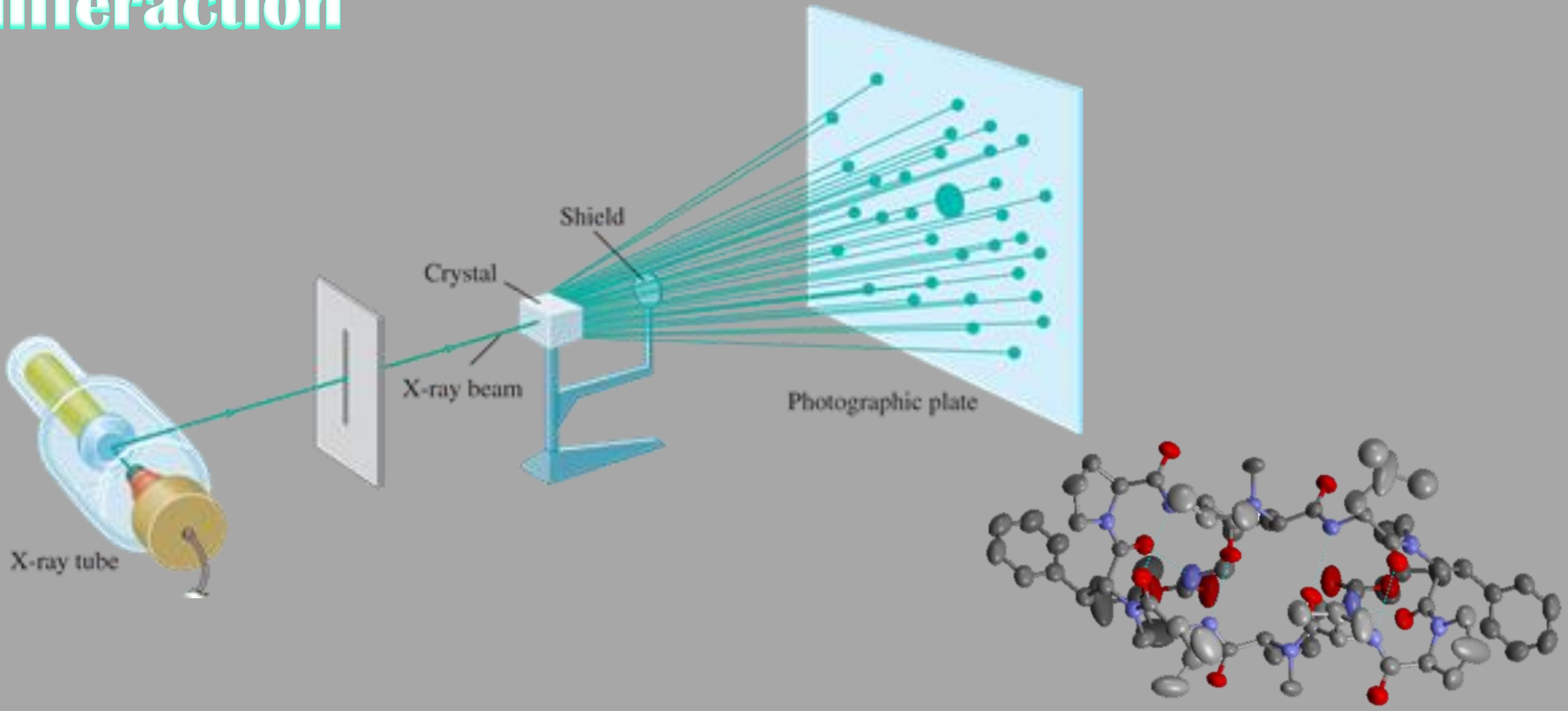
Types of carbon are present?

Carbon bumber of each type.



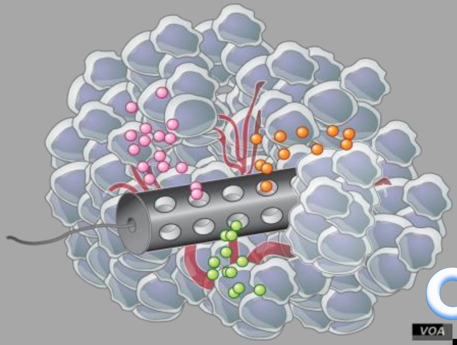
X-Ray Spectroscopy

Identification of the 3D structure of any compound present in crystal form by X-Ray differaction



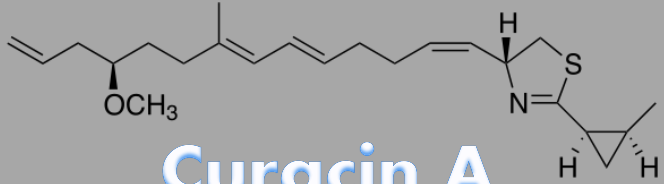
Structure with Stereochemistry

Bioactive Compounds in Clinical Trials



Bioactive Compounds

Clinical Trials



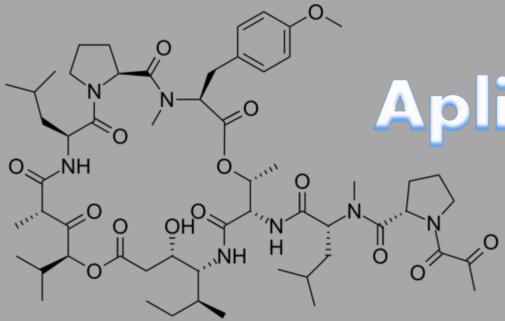
Curacin A

Succeed

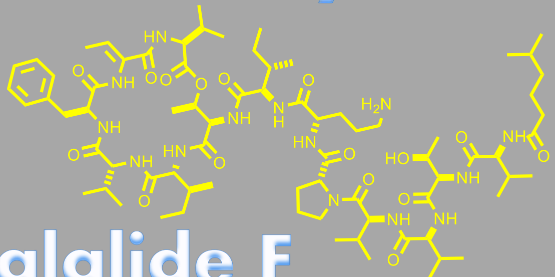
- ☐ Approved
- ☐ 30 – 40 years
- ☐ 1 Billion USD

Fail

- ☐ Unstable
- ☐ Toxic
- ☐ Insufficient Supply
- ☐ Difficult synthesis



Aplidin



kahalalide F

Thank You